



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 01:46 PM UTC

PDB ID : 6HIZ / pdb_00006hiz
EMDB ID : EMD-0233
Title : Cryo-EM structure of the Trypanosoma brucei mitochondrial ribosome - This entry contains the head of the small mitoribosomal subunit
Authors : Ramrath, D.J.F.; Niemann, M.; Leibundgut, M.; Bieri, P.; Prange, C.; Horn, E.K.; Leitner, A.; Boehringer, A.; Schneider, A.; Ban, N.
Deposited on : 2018-08-31
Resolution : 3.08 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

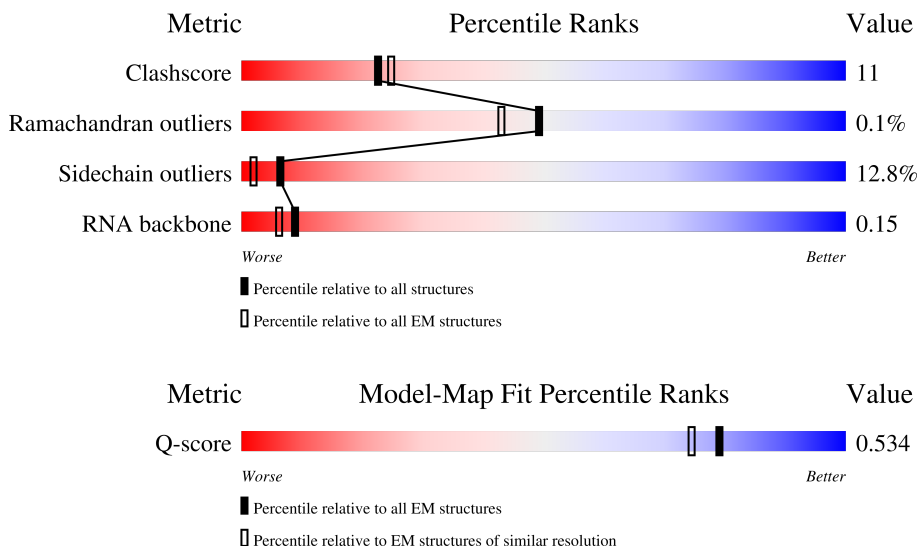
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



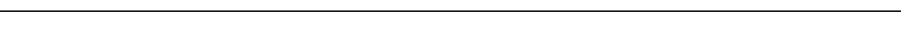
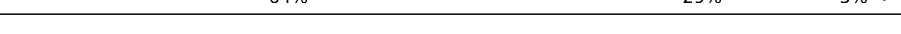
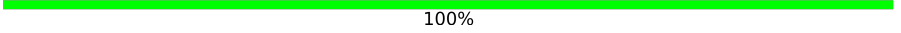
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14000 (2.58 - 3.58)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	DA	1788	
2	DL	307	
3	DB	1181	

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Mol	Chain	Length	Quality of chain
4	DC	1165	
5	DE	747	
6	DF	666	
7	DG	631	
8	DH	581	
9	DJ	396	
10	DK	324	
11	DT	247	
12	DV	183	
13	DW	179	
14	DX	169	
15	DY	163	
16	CC	74	
17	CI	443	
18	CJ	817	
19	CK	326	
20	CN	166	
21	CR	320	
22	CS	244	
23	Cg	498	
24	Ci	181	
25	Ck	874	
26	CA	611	
27	UO	5	
28	UP	7	

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 76845 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called mS48.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	DA	131	Total	C	N	O	S	0	0
			993	629	174	186	4		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	894	HIS	ASN	conflict	UNP Q57UJ2
DA	1181	THR	ILE	conflict	UNP Q57UJ2
DA	1333	ALA	VAL	conflict	UNP Q57UJ2
DA	1700	ARG	HIS	conflict	UNP Q57UJ2
DA	1761	LYS	ARG	conflict	UNP Q57UJ2

- Molecule 2 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	DL	143	Total	C	N	O	S	0	0
			1153	733	215	202	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DL	274	THR	ALA	conflict	UNP Q38BS2

- Molecule 3 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	DB	1111	Total	C	N	O	S	0	0
			9148	5691	1717	1711	29		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DB	23	VAL	ALA	conflict	UNP Q586P5

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Chain	Residue	Modelled	Actual	Comment	Reference
DB	359	ILE	THR	conflict	UNP Q586P5
DB	384	GLN	HIS	conflict	UNP Q586P5
DB	402	THR	ILE	conflict	UNP Q586P5
DB	423	THR	ALA	conflict	UNP Q586P5
DB	586	ARG	HIS	conflict	UNP Q586P5
DB	593	ARG	LYS	conflict	UNP Q586P5
DB	647	SER	GLY	conflict	UNP Q586P5

- Molecule 4 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	DC	1095	Total	C	N	O	S	0	0
			8748	5519	1544	1654	31		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	53	ALA	THR	conflict	UNP Q57YB5
DC	365	LYS	GLU	conflict	UNP Q57YB5
DC	385	THR	ALA	conflict	UNP Q57YB5
DC	405	ILE	VAL	conflict	UNP Q57YB5
DC	641	SER	PRO	conflict	UNP Q57YB5
DC	651	LYS	GLU	conflict	UNP Q57YB5
DC	731	GLU	ASP	conflict	UNP Q57YB5
DC	814	GLN	HIS	conflict	UNP Q57YB5
DC	1097	ALA	VAL	conflict	UNP Q57YB5
DC	1113	THR	ILE	conflict	UNP Q57YB5

- Molecule 5 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	DE	590	Total	C	N	O	S	0	0
			4831	3075	874	863	19		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DE	514	THR	SER	conflict	UNP Q386Q7

- Molecule 6 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	DF	590	Total	C	N	O	S	0	0
			4747	2979	896	847	25		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DF	18	THR	ALA	conflict	UNP Q38ET1
DF	258	ASP	ASN	conflict	UNP Q38ET1
DF	372	ASN	ASP	conflict	UNP Q38ET1
DF	406	ASN	SER	conflict	UNP Q38ET1
DF	510	ASP	GLY	conflict	UNP Q38ET1
DF	577	ALA	VAL	conflict	UNP Q38ET1
DF	636	UNK	GLY	conflict	UNP Q38ET1
DF	638	LYS	ARG	conflict	UNP Q38ET1

- Molecule 7 is a protein called mS54.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	DG	566	Total	C	N	O	S	0	0
			4575	2875	835	834	31		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DG	428	ASN	SER	conflict	UNP Q57ZP8
DG	429	GLY	SER	conflict	UNP Q57ZP8

- Molecule 8 is a protein called mS55.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	DH	564	Total	C	N	O	S	0	0
			4578	2872	850	834	22		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DH	191	HIS	GLN	conflict	UNP Q580V1
DH	194	PRO	ARG	conflict	UNP Q580V1
DH	488	GLY	SER	conflict	UNP Q580V1

- Molecule 9 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	DJ	315	Total	C	N	O	S	0	0
			2572	1646	452	460	14		

- Molecule 10 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	DK	255	Total	C	N	O	S	0	0
			2007	1260	365	377	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DK	61	SER	PRO	conflict	UNP Q38BP1
DK	257	GLY	SER	conflict	UNP Q38BP1

- Molecule 11 is a protein called mS67.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	DT	239	Total	C	N	O	S	0	0
			2058	1321	364	362	11		

- Molecule 12 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	DV	160	Total	C	N	O	S	0	0
			1346	855	252	235	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DV	163	ALA	THR	conflict	UNP Q57UZ6

- Molecule 13 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	DW	161	Total	C	N	O	S	0	0
			1359	866	260	228	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DW	74	THR	MET	conflict	UNP Q383N9

- Molecule 14 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	DX	141	Total	C	N	O	S	0	0
			1196	762	226	201	7		

- Molecule 15 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	DY	154	Total	C	N	O	S	0	0
			1293	827	245	216	5		

- Molecule 16 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CC	74	Total	C	N	O	S	0	0
			646	451	96	98	1		

- Molecule 17 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CI	222	Total	C	N	O	S	0	0
			1754	1101	330	313	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	279	UNK	ARG	conflict	UNP Q57W62
CI	370	ALA	VAL	conflict	UNP Q57W62

- Molecule 18 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CJ	800	Total	C	N	O	S	0	0
			6516	4119	1151	1216	30		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	311	LEU	TYR	conflict	UNP Q57Z45
CJ	484	HIS	ARG	conflict	UNP Q57Z45
CJ	488	SER	ASN	conflict	UNP Q57Z45
CJ	594	GLU	VAL	conflict	UNP Q57Z45

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Chain	Residue	Modelled	Actual	Comment	Reference
CJ	629	ARG	LYS	conflict	UNP Q57Z45

- Molecule 19 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CK	52	Total	C	N	O	S	0	0
			438	272	90	74	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CK	3	ARG	GLN	conflict	UNP Q389T7
CK	138	UNK	ILE	conflict	UNP Q389T7

- Molecule 20 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CN	157	Total	C	N	O	S	0	0
			1322	843	251	220	8		

- Molecule 21 is a protein called uS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CR	44	Total	C	N	O	S	0	0
			353	217	64	71	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CR	8	ILE	VAL	conflict	UNP Q38AS2

- Molecule 22 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CS	142	Total	C	N	O	S	0	0
			1175	761	210	198	6		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CS	-71	MET	-	initiating methionine	UNP Q584T8

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Chain	Residue	Modelled	Actual	Comment	Reference
CS	-70	ALA	-	expression tag	UNP Q584T8
CS	-69	PHE	-	expression tag	UNP Q584T8
CS	-68	ARG	-	expression tag	UNP Q584T8
CS	-67	ASN	-	expression tag	UNP Q584T8
CS	-66	THR	-	expression tag	UNP Q584T8
CS	-65	PHE	-	expression tag	UNP Q584T8
CS	-64	THR	-	expression tag	UNP Q584T8
CS	-63	THR	-	expression tag	UNP Q584T8
CS	-62	PRO	-	expression tag	UNP Q584T8
CS	-61	GLY	-	expression tag	UNP Q584T8
CS	-60	LYS	-	expression tag	UNP Q584T8
CS	-59	PHE	-	expression tag	UNP Q584T8
CS	-58	SER	-	expression tag	UNP Q584T8
CS	-57	THR	-	expression tag	UNP Q584T8
CS	-56	VAL	-	expression tag	UNP Q584T8
CS	-55	SER	-	expression tag	UNP Q584T8
CS	-54	LYS	-	expression tag	UNP Q584T8
CS	-53	ASN	-	expression tag	UNP Q584T8
CS	-52	ILE	-	expression tag	UNP Q584T8
CS	-51	VAL	-	expression tag	UNP Q584T8
CS	-50	LEU	-	expression tag	UNP Q584T8
CS	-49	LEU	-	expression tag	UNP Q584T8
CS	-48	LEU	-	expression tag	UNP Q584T8
CS	-47	ILE	-	expression tag	UNP Q584T8
CS	-46	TRP	-	expression tag	UNP Q584T8
CS	-45	ARG	-	expression tag	UNP Q584T8
CS	-44	VAL	-	expression tag	UNP Q584T8
CS	-43	LYS	-	expression tag	UNP Q584T8
CS	-42	VAL	-	expression tag	UNP Q584T8
CS	-41	PHE	-	expression tag	UNP Q584T8
CS	-40	LEU	-	expression tag	UNP Q584T8
CS	-39	ARG	-	expression tag	UNP Q584T8
CS	-38	ALA	-	expression tag	UNP Q584T8
CS	-37	GLU	-	expression tag	UNP Q584T8
CS	-36	GLY	-	expression tag	UNP Q584T8
CS	-35	PHE	-	expression tag	UNP Q584T8
CS	-34	ALA	-	expression tag	UNP Q584T8
CS	-33	HIS	-	expression tag	UNP Q584T8
CS	-32	SER	-	expression tag	UNP Q584T8
CS	-31	LEU	-	expression tag	UNP Q584T8
CS	-30	VAL	-	expression tag	UNP Q584T8
CS	-29	MET	-	expression tag	UNP Q584T8

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Chain	Residue	Modelled	Actual	Comment	Reference
CS	-28	LEU	-	expression tag	UNP Q584T8
CS	-27	PRO	-	expression tag	UNP Q584T8
CS	-26	VAL	-	expression tag	UNP Q584T8
CS	-25	SER	-	expression tag	UNP Q584T8
CS	-24	LEU	-	expression tag	UNP Q584T8
CS	-23	TYR	-	expression tag	UNP Q584T8
CS	-22	SER	-	expression tag	UNP Q584T8
CS	-21	LYS	-	expression tag	UNP Q584T8
CS	-20	ILE	-	expression tag	UNP Q584T8
CS	-19	LEU	-	expression tag	UNP Q584T8
CS	-18	LEU	-	expression tag	UNP Q584T8
CS	-17	CYS	-	expression tag	UNP Q584T8
CS	-16	ASP	-	expression tag	UNP Q584T8
CS	-15	VAL	-	expression tag	UNP Q584T8
CS	-14	LYS	-	expression tag	UNP Q584T8
CS	-13	LYS	-	expression tag	UNP Q584T8
CS	-12	LYS	-	expression tag	UNP Q584T8
CS	-11	ILE	-	expression tag	UNP Q584T8
CS	-10	VAL	-	expression tag	UNP Q584T8
CS	-9	TYR	-	expression tag	UNP Q584T8
CS	-8	PHE	-	expression tag	UNP Q584T8
CS	-7	HIS	-	expression tag	UNP Q584T8
CS	-6	CYS	-	expression tag	UNP Q584T8
CS	-5	CYS	-	expression tag	UNP Q584T8
CS	-4	THR	-	expression tag	UNP Q584T8
CS	-3	ARG	-	expression tag	UNP Q584T8
CS	-2	LYS	-	expression tag	UNP Q584T8
CS	-1	LYS	-	expression tag	UNP Q584T8
CS	0	SER	-	expression tag	UNP Q584T8

- Molecule 23 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Cg	482	Total	C	N	O	S	0	0
			3904	2499	684	701	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cg	181	VAL	ALA	conflict	UNP Q585C2
Cg	498	ARG	MET	conflict	UNP Q585C2

- Molecule 24 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ci	165	Total	C	N	O	S	0	0
			1348	848	247	244	9		

- Molecule 25 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ck	703	Total	C	N	O	S	0	0
			5596	3503	1017	1050	26		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ck	107	SER	LEU	conflict	UNP Q387C7
Ck	144	PHE	LEU	conflict	UNP Q387C7
Ck	253	TYR	PHE	conflict	UNP Q387C7
Ck	339	GLU	VAL	conflict	UNP Q387C7
Ck	871	GLY	GLU	conflict	UNP Q387C7

- Molecule 26 is a RNA chain called RNA (143-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CA	143	Total	C	N	O	P	0	0
			3030	1364	522	1001	143		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	473	U	G	conflict	GB 343546

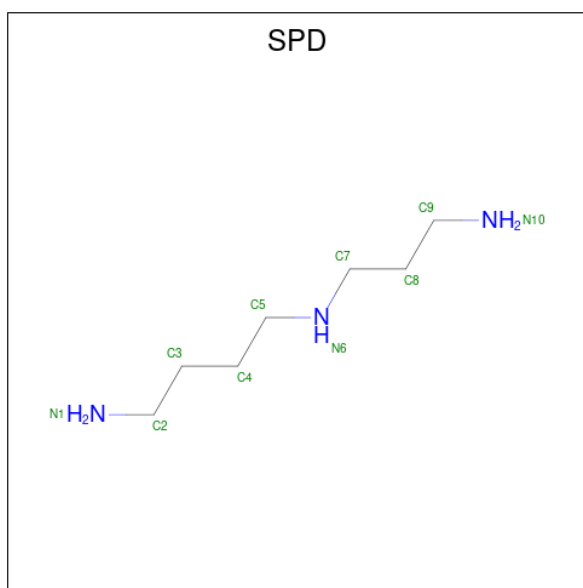
- Molecule 27 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	UO	5	Total	C	N	O	0	0
			30	20	5	5		

- Molecule 28 is a protein called Unknown protein.

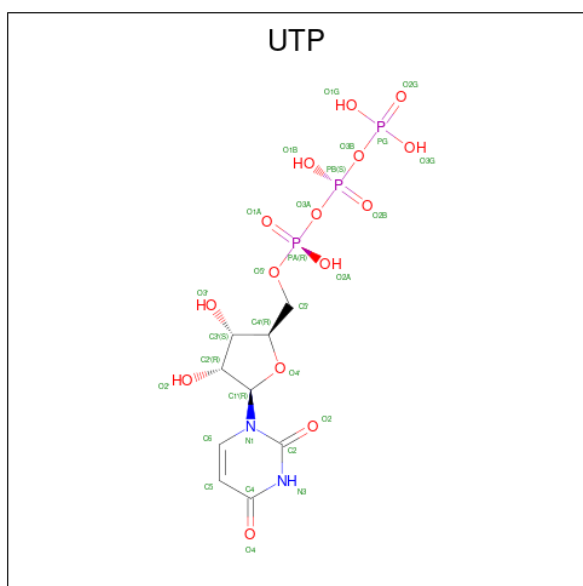
Mol	Chain	Residues	Atoms				AltConf	Trace
28	UP	7	Total	C	N	O	0	0
			42	28	7	7		

- Molecule 29 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



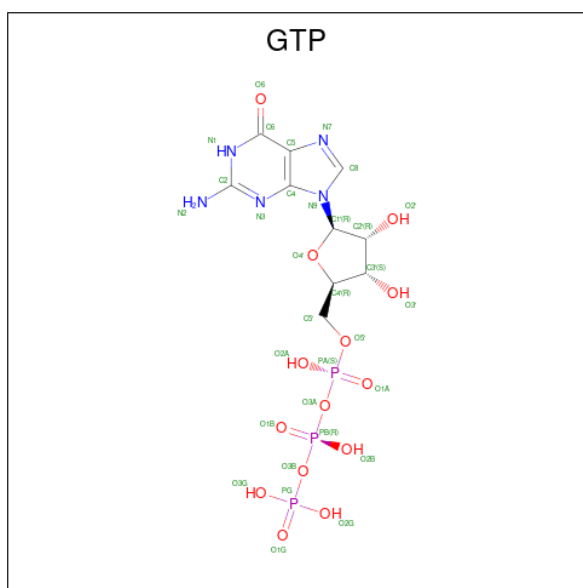
Mol	Chain	Residues	Atoms			AltConf
29	DL	1	Total	C	N	0
			10	7	3	
29	CA	1	Total	C	N	0
			10	7	3	

- Molecule 30 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).



Mol	Chain	Residues	Atoms					AltConf
30	DJ	1	Total	C	N	O	P	0
			29	9	2	15	3	

- Molecule 31 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
31	Cg	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	Cg	1	Total	Mg	0
			1	1	
32	CA	2	Total	Mg	0
			2	2	

- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	Cg	3	Total	O	0
			3	3	

PRO	LEU	PHE	GLN	ARG	PHE	GLU	ARG	GLY	LEU	LEU	LEU	GLU	PRO	ARG	ALA	ASN	LEU	LYS	PHE	PHE	THR	SER	ARG	ALA	SER	GLN	GLN	SER	THR	GLN	LEU	GLY	ARG	ARG	G266	H267	M268	M269	T270	P271	H272	T273	T274	L275	H276	G277	R278	W282	T286	W287	L294	G295	P296	P302	G303	M304	T305	P306	ASP
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• Molecule 3: mS49

Chain DB:  66% 23% 5% 6%

MET	ILE	ARG	ARG	GLY	ASN	VAL	CYS	ASP	GLY	ALA	ARG	LEU	GLU	W72	R78	A91	H92	K93	D94	D98	V99	Q220	H221	R110	M114	G115	G116	A117	V118	A119	P121	H122	I123	E128	Y129	E130	E131	V137	W138	L139	D140	H141	R145	M146	H153	R154	L157	R173	V183
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THR	ALA	GLY	GLU	ASN	PRO	ALA	SER	SER	GLY	D71	W72	R78	A91	H92	K93	D94	D98	V99	Q220	H221	R110	M114	G115	G116	A117	V118	A119	P121	H122	I123	E128	Y129	E130	E131	V137	W138	L139	D140	H141	R145	M146	H153	R154	L157	R173	V183
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S186	V189	H190	I192	I193	Q194	S204	A205	L206	Q209	R214	I217	A218	E219	Q220	H221	T228	D231	R232	D233	D236	S249	L255	V276	Q281	M285	T295	Q301	L302	P303	P308	S309	L318	S321	T326	P327	A333
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R339	T341	V342	Q355	I357	N358	I359	T365	E368	G382	A386	L387	V388	Q389	D394	Q395	T397	K400	T402	N403	F413	O414	Q415	N416	T423	D424	K427	N428	P429	R433	S434	T435	E436	V439	O440	N445	D448	T449	M450
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R451	R452	E453	D454	R455	L456	Q461	D462	L463	T464	E465	Y471	G472	V473	P474	L478	V479	V483	H486	R487	N488	R490	R493	P494	L495	L507	N510	R511	Y513	R514	E517	G518	F519	S520	M522	P526	E527	F528	L529	E532	Q539	R544	R545	R546
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L547	A548	L549	L550	H551	G552	L553	E554	A557	N558	E559	T560	A561	Q562	R564	H569	D572	E573	L574	F580	E584	M585	R586	V587	N588	D589	D590	E591	M592	E597	L608	P609	V614	A622	S623	L626	M635	G636	T637	R641	S646	G647	R648	L656
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R662	V663	G664	R665	V671	V672	Q684	P685	Q686	L689	S693	E716	M719	K720	R722	Y731	V735	V743	V744	L755	T756	V757	S758	E765	A768	V769	N774	T776	V783	Y784	N785	L786	L787	P788	N789	S790	R793	Y794	V795	P796	Q800	L801
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D802	E805	T810	D815	R816	E820	P823	L826	L830	N831	Y832	G833	T834	Y837	R841	D849	S850	T851	M852	G859	Q860	R861	T867	H868	L876	P877	V878	R881	P885	Q891	R892	L893	Q898	Y901	I902	I903	Q904	Y905	Q908	P909	F910
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L917	V918	V920	A921	F922	Q923	M929	E930	R939	M937	Q940	R941	H944	G945	P946	R948	T949	V950	S954	R955	N958	P959	M962	R963	R964	V968	T969	K975	H981	L983	D984	R990	D993	T994	V995	T1001	T1002	Q1005	I1005	D1009	T1012	R1013
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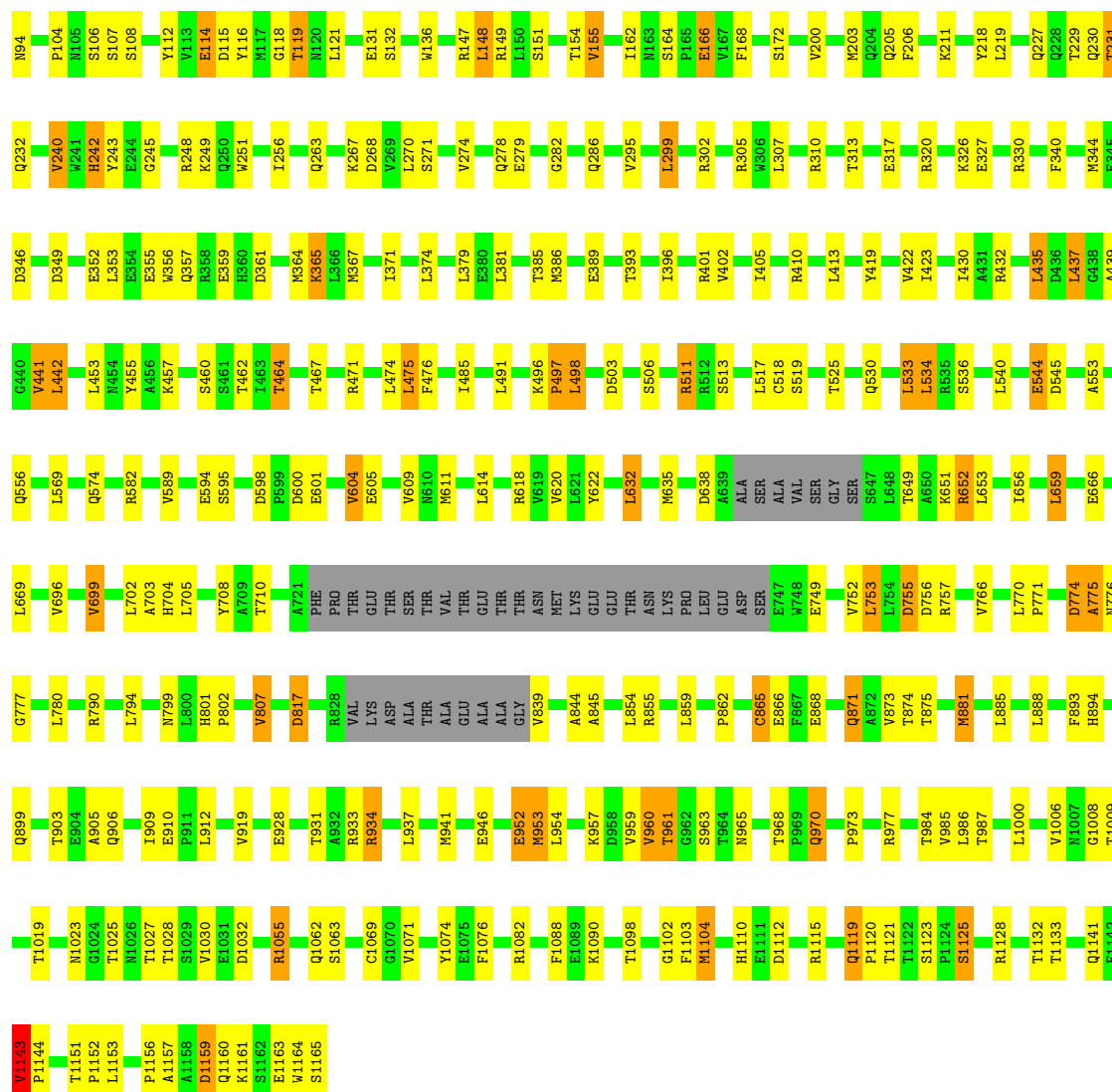
D1020	R1023	S1026	T1027	S1028	R1029	R1030	R1031	D1032	Y1033	I1034	Q1035	E1036	I1039	Y1042	T1043	P1044	V1047	Q1051	A1052	A1053	Q1054	Q1055	P1056	D1065	M1066	T1067	G1068	T1069	V1079	R1080	Y1081	K1082	L1100	Q1101	Y1102	V1103	D1104	G1105	V1106	T1107	P1108	W1109	K1110	T1117	H1125	P1126	M1127
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R1132	P1133	E1134	V1135	A1136	M1137	V1142	G1143	L1144	L1145	P1146	D1153	T1156	G1157	K1158	V1159	K1160	D1164	S1165	V1166	R1167	D1168	K1172	T1173	L1181
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• Molecule 4: mS50

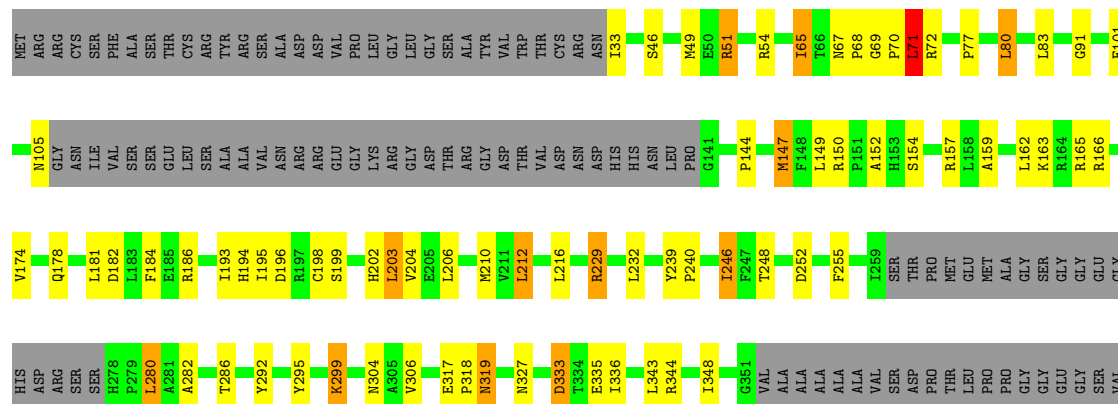
Chain DC:  67% 23% 5% 6%

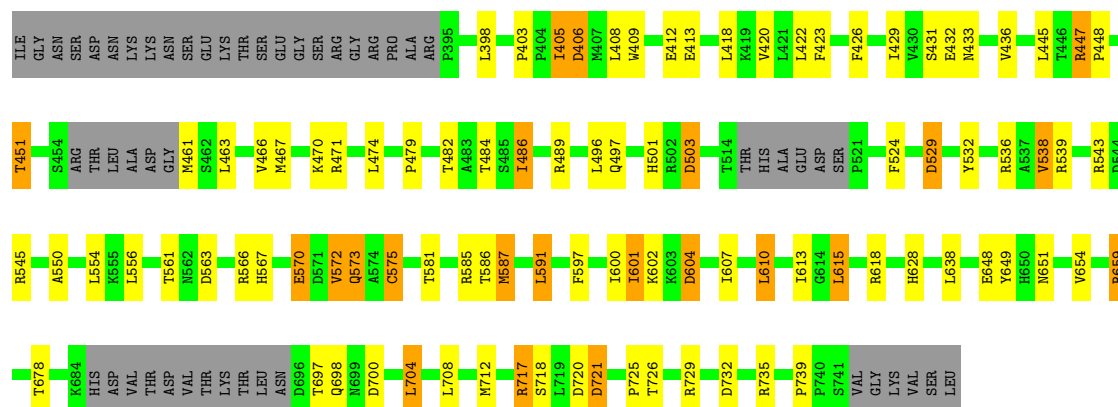
MET	PHE	ARG	VAL	ARG	ARG	LEU	ALA	GLY	PHE	ILE	GLN	CYS	SER	PRO	CYS	GLY	LYS	MET	GLY	PRO	LEU	LYS	GLN	THR	ARG	Y29	T30	D36	R46	E50	A56	E57	V58	I61	W71	D77	P78	H81	T82	P85	T86	M87	L88	G89	G90	K91	F92	R93
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• Molecule 5: mS52

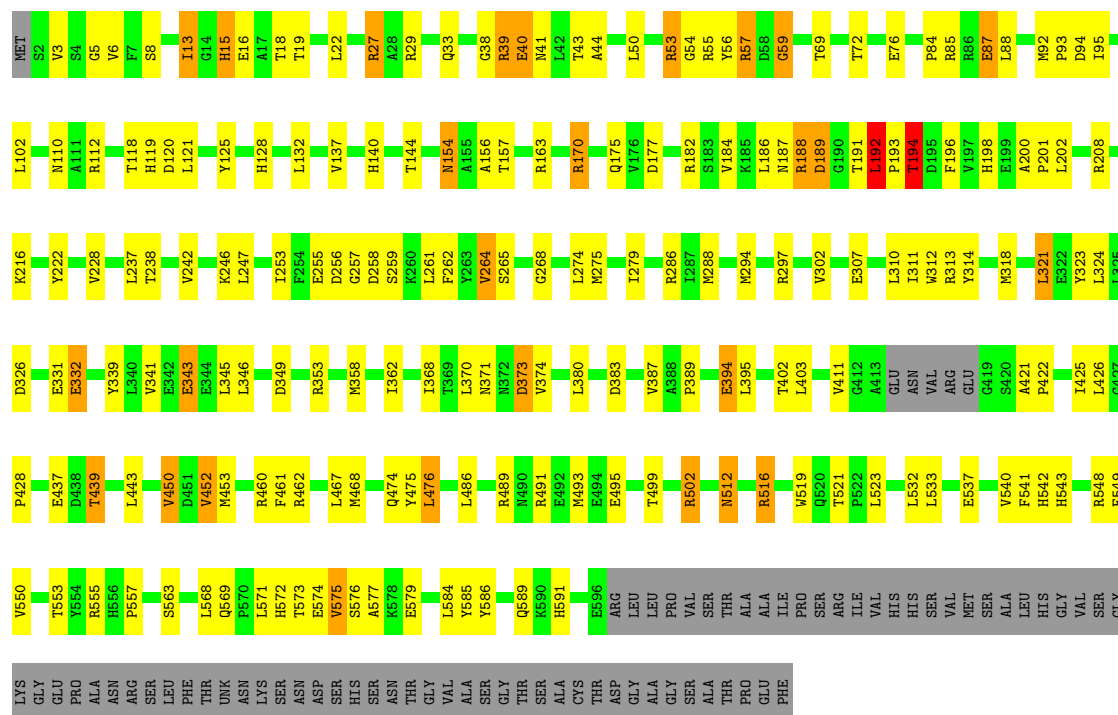
Chain DE: 56% 18% 5% 21%





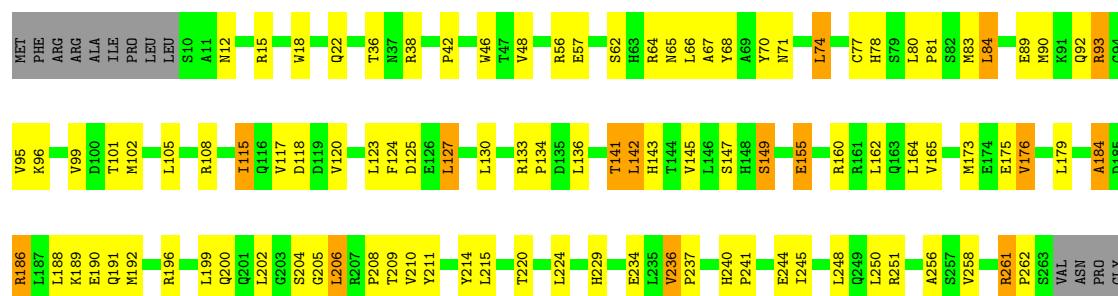
• Molecule 6: mS53

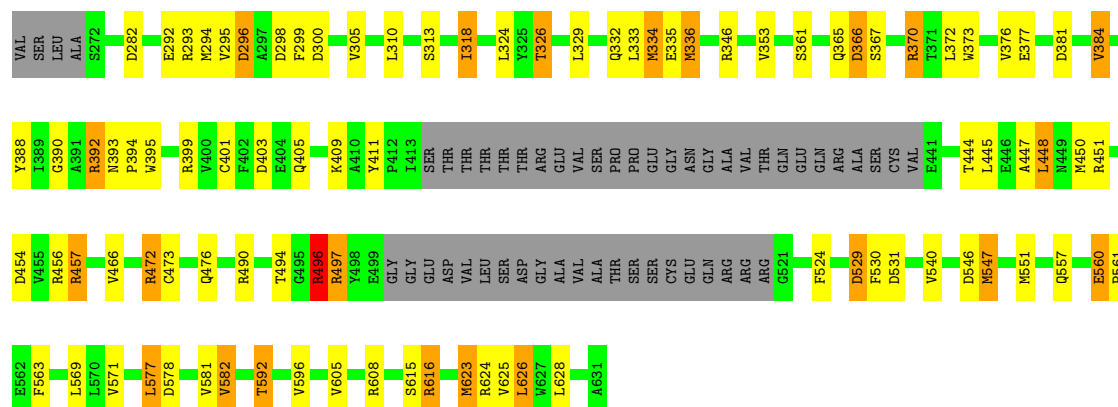
Chain DF: 59% 25% 11%



• Molecule 7: mS54

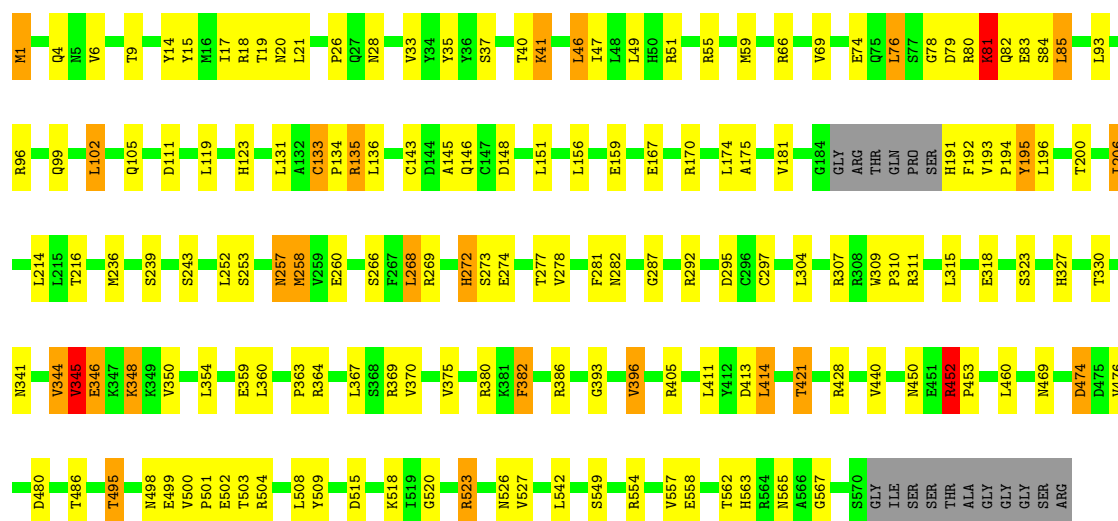
Chain DG: 59% 25% 6% 10%





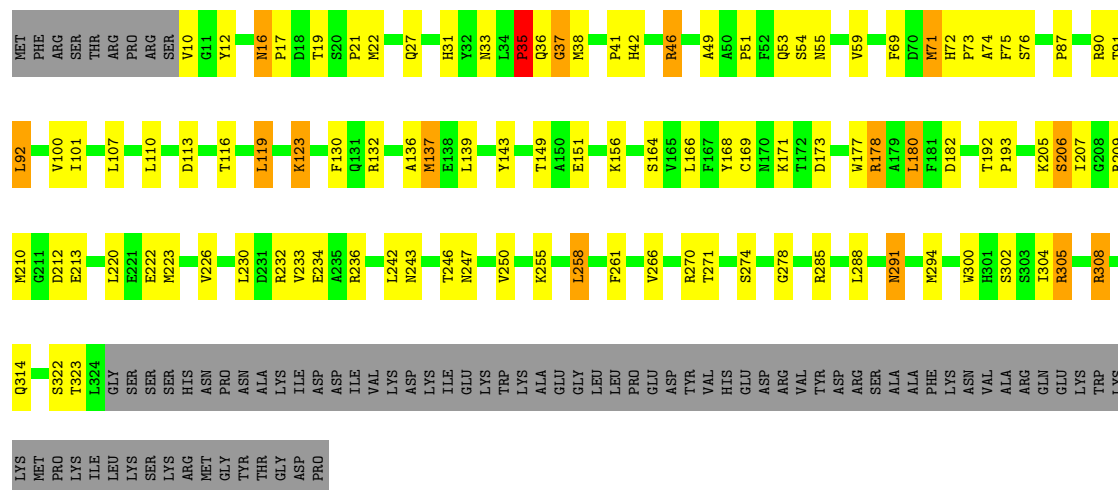
• Molecule 8: mS55

Chain DH: 69% 24%



• Molecule 9: mS57

Chain DJ: 53% 22% 20%



777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000
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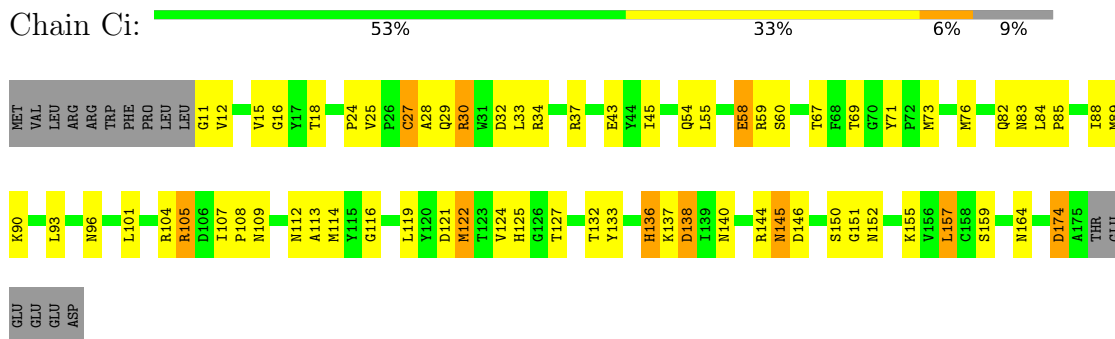
T93	T96	Q99	E102	Q106	F109	T110	R111	H112	V113	T124	T125	Q128	D133	Y138	V141	R148	R161	R162	K163																											
MET	LEU	ARG	SER	THR	LEU	THR	SER	LEU	R10	T11	T14	S15	P20	S23	W32	A33	D34	P35	E36	R37	M38	V39	R40	L43	T47	L48	G49	V50	D51	Q52	L53	P54	T58	Q62	R63	D64	L65	C71	V77	G78	D79	S80	T81	K84	R87	T92

M4
 I7
 V10
 T14
 I15
 L16
 Q17
 K18
 Y19
 T20
 F21
 K22
 L36
 L44
 L45
 W46
 L47
 I50
 H51
 I52
 I55
 F62
 L65
 N66
 N67
 F68
 E69
 Y70
 L71
 I72
 I73
 L74
 I75
 S76
 T77

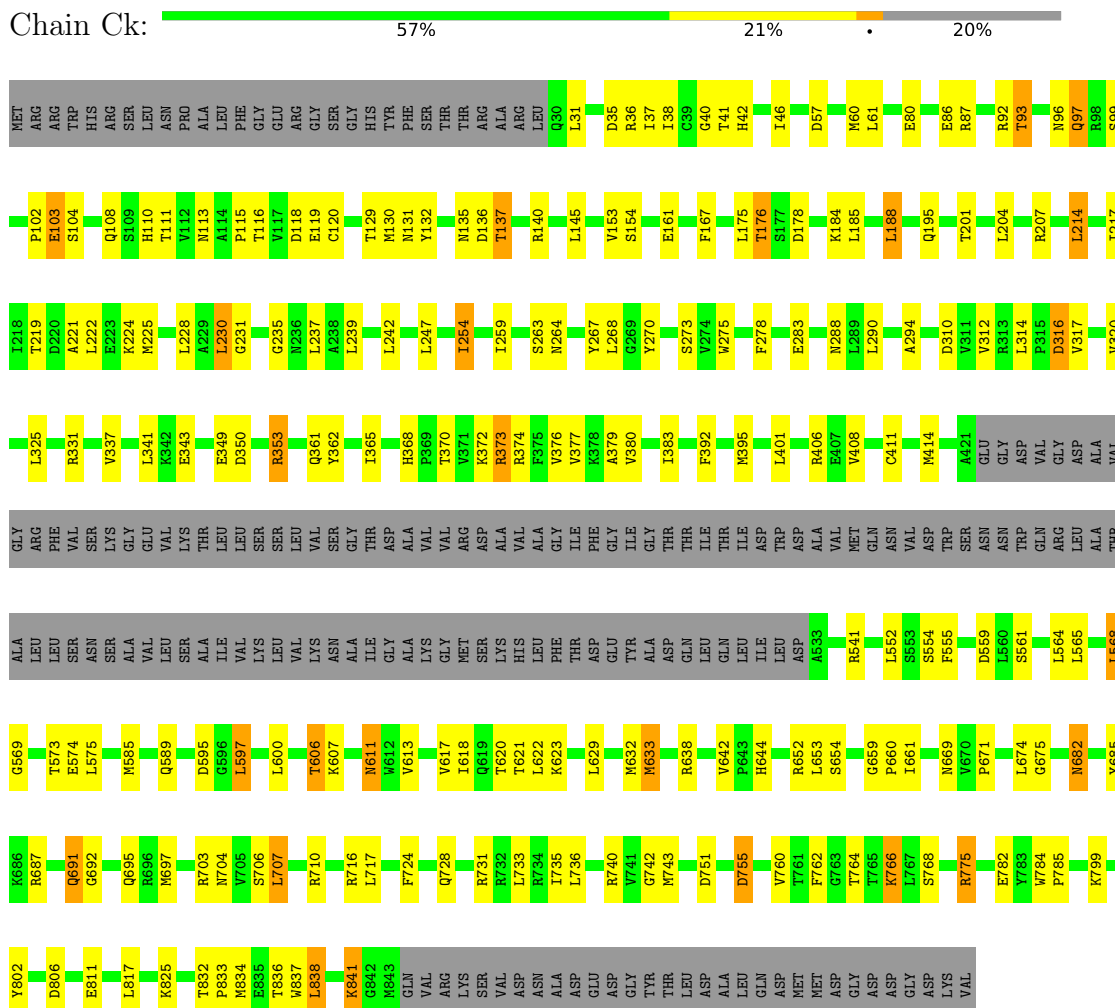
M356	M366	PHE	THR	ASN	THR	ALA	GLU	M1
A361	Q2	THR	PHE	GLN	GLU	GLN	TYR	Q2
I372	L4	VAL	LEU	ILE	ILE	ILE	PRO	K3
E375	T9	LEU	GLU	GLY	GLY	GLY	MET	L4
R392	A10	LYS	TRP	THR	THR	THR	TYR	T9
V400	A10	ASP	MET	VAL	VAL	VAL	PRO	A10
T406	R14	PHE	GLY	LEU	LEU	LEU	GLY	R14
R407	F16	ALA	ARG	ALA	ALA	ALA	TYR	F16
L410	L15	UNK	THR	LEU	LEU	LEU	PRO	L15
K411	R17	VAL	GLU	PHE	PHE	PHE	ALA	R17
K412	L18	ALA	THR	THR	THR	THR	ALA	L18
L415	K32	ALA	HIS	HIS	HIS	HIS	HIS	K32
R420	S33	ASP	PHE	ASN	ASN	ASN	THR	S33
R421	D34	GLU	ALA	LEU	LEU	LEU	LEU	D34
R422	G35	ARG	THR	TYR	TYR	TYR	SER	G35
L431	E36	HIS	GLU	GLU	GLU	GLU	SER	E36
K435	R37	Q289	HIS	HIS	HIS	HIS	LEU	R37
V436	L38	T290	ALA	ALA	ALA	ALA	ARG	L38
R439	V39	R293	LEU	LEU	LEU	LEU	ASP	V39
R443	R40	T294	PHE	PHE	PHE	PHE	GLU	R40
	V41	D295	GLU	GLU	GLU	GLU	LEU	V41
	R42	T303	PHE	SER	SER	SER	ARG	R42
	S43	G304	ARG	ARG	ARG	ARG	ASP	S43
	S54	I305	LYS	LYS	LYS	LYS	THR	S54
E57	E57	A306	PHE	PHE	PHE	PHE	THR	E57
E58	R59	V307	ASN	ASN	ASN	ASN	GLY	R59
E62	E62	G308	ARG	ARG	ARG	ARG	LEU	E62
R65	R65	R309	ASP	ASP	ASP	ASP	VAL	R65
P66	P66	G310	VAL	VAL	VAL	VAL	GLY	P66
L67	L67	A311	ARG	ARG	ARG	ARG	ALA	L67
GLU	GLU	D313	VAL	VAL	VAL	VAL	SER	GLU
VAL	VAL	E315	MET	MET	MET	MET	ARG	VAL
GLY	GLY	T320	PHE	PHE	PHE	PHE	GLY	GLY
GLU	GLU	A321	ASN	ASN	ASN	ASN	GLN	GLU
ASN	ASN	L322	THR	THR	THR	THR	LEU	ASN
SER	SER	L323	ARG	ARG	ARG	ARG	GLY	SER
PHE	PHE	R324	LEU	LEU	LEU	LEU	VAL	PHE
ALA	ALA	E325	MET	MET	MET	MET	THR	ALA
ALA	ALA	N326	SER	SER	SER	SER	ILE	ALA
ASN	ASN		LYS	LYS	LYS	LYS	THR	ASN
GLY	GLY	R330	ALA	ALA	ALA	ALA	ALA	GLY
GLN	GLN	G331	THR	THR	THR	THR	GLU	GLN
ALA	ALA	I332	LEU	LEU	LEU	LEU	ALA	ALA
THR	THR		ALA	ALA	ALA	ALA	GLY	THR
HIS	HIS	K338	ASP	ASP	ASP	ASP	LEU	HIS
GLY	GLY		SER	SER	SER	SER	ASP	GLY
ASN	ASN	V343	ALA	ALA	ALA	ALA	ASN	ASN
ASN	ASN		ASP	ASP	ASP	ASP	ALA	ASN
PHE	PHE	K351	SER	SER	SER	SER	PRO	PHE
TYR	TYR	E352	THR	THR	THR	THR	GLY	TYR
ARG	ARG	K353	SER	SER	SER	SER	LEU	ARG

Chain CJ: 64% 29% 5%

- Molecule 24: mS33



- Molecule 25: mS35



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101308	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.587	Depositor
Minimum map value	-0.258	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, GTP, UTP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	DA	0.45	0/1010	0.90	5/1369 (0.4%)
2	DL	0.58	0/1185	1.01	5/1601 (0.3%)
3	DB	0.56	0/9369	0.98	30/12692 (0.2%)
4	DC	0.52	0/8952	0.93	23/12145 (0.2%)
5	DE	0.51	0/4955	0.97	17/6708 (0.3%)
6	DF	0.57	0/4856	0.96	13/6581 (0.2%)
7	DG	0.48	0/4674	0.92	6/6333 (0.1%)
8	DH	0.58	0/4684	0.96	16/6347 (0.3%)
9	DJ	0.57	1/2649 (0.0%)	0.97	6/3598 (0.2%)
10	DK	0.57	0/2045	0.92	2/2759 (0.1%)
11	DT	0.61	0/2133	1.03	7/2889 (0.2%)
12	DV	0.61	0/1382	1.06	5/1871 (0.3%)
13	DW	0.51	0/1407	0.95	4/1916 (0.2%)
14	DX	0.56	0/1231	1.02	9/1654 (0.5%)
15	DY	0.64	0/1334	0.98	3/1810 (0.2%)
16	CC	0.63	0/666	1.09	2/900 (0.2%)
17	CI	0.59	0/1783	1.00	2/2395 (0.1%)
18	CJ	0.67	3/6705 (0.0%)	1.06	49/9124 (0.5%)
19	CK	0.49	0/448	0.91	0/600
20	CN	0.63	0/1361	0.99	4/1840 (0.2%)
21	CR	0.55	0/361	1.18	5/490 (1.0%)
22	CS	0.55	0/1209	1.05	12/1626 (0.7%)
23	Cg	0.56	0/4025	1.00	15/5467 (0.3%)
24	Ci	0.67	0/1388	1.09	4/1878 (0.2%)
25	Ck	0.54	0/5696	0.94	6/7705 (0.1%)
26	CA	0.34	0/3392	0.52	0/5275
All	All	0.56	4/78900 (0.0%)	0.96	250/107573 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	DL	0	2
3	DB	0	2
4	DC	0	2
7	DG	0	2
9	DJ	0	1
11	DT	0	1
14	DX	0	1
18	CJ	0	1
23	Cg	0	1
24	Ci	0	1
25	Ck	0	1
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	CJ	424	HIS	CG-CD2	-12.76	1.21	1.35
18	CJ	424	HIS	CD2-NE2	9.05	1.47	1.37
18	CJ	424	HIS	CG-ND1	7.88	1.47	1.38
9	DJ	255	LYS	C-O	5.84	1.30	1.24

The worst 5 of 250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DH	133	CYS	CA-C-N	-10.96	106.13	119.84
8	DH	133	CYS	C-N-CA	-10.96	106.13	119.84
5	DE	327	ASN	CA-C-N	-10.94	109.11	120.38
5	DE	327	ASN	C-N-CA	-10.94	109.11	120.38
18	CJ	783	ILE	CA-C-N	10.31	130.41	120.31

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	DB	383	ARG	Sidechain
3	DB	586	ARG	Sidechain
4	DC	497	PRO	Peptide
2	DL	269	MET	Peptide
2	DL	270	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DA	993	0	1016	21	0
2	DL	1153	0	1146	33	0
3	DB	9148	0	8834	228	0
4	DC	8748	0	8532	190	0
5	DE	4831	0	4789	110	0
6	DF	4747	0	4723	155	0
7	DG	4575	0	4490	150	0
8	DH	4578	0	4520	128	0
9	DJ	2572	0	2495	81	0
10	DK	2007	0	1998	46	0
11	DT	2058	0	1928	60	0
12	DV	1346	0	1335	47	0
13	DW	1359	0	1342	44	0
14	DX	1196	0	1189	41	0
15	DY	1293	0	1287	39	0
16	CC	646	0	679	19	0
17	CI	1754	0	1806	41	0
18	CJ	6516	0	6261	199	0
19	CK	438	0	438	13	0
20	CN	1322	0	1304	42	0
21	CR	353	0	334	13	0
22	CS	1175	0	1191	46	0
23	Cg	3904	0	3785	95	0
24	Ci	1348	0	1306	56	0
25	Ck	5596	0	5613	153	0
26	CA	3030	0	1513	52	0
27	UO	30	0	33	0	0
28	UP	42	0	44	0	0
29	CA	10	0	19	2	0
29	DL	10	0	19	0	0
30	DJ	29	0	11	5	0
31	Cg	32	0	12	7	0
32	CA	2	0	0	0	0
32	Cg	1	0	0	0	0
33	Cg	3	0	0	1	0
All	All	76845	0	73992	1698	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1698 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CJ:484:HIS:CD2	18:CJ:495:ARG:NH1	1.87	1.42
18:CJ:544:THR:CG2	18:CJ:552:ILE:HG12	1.53	1.36
18:CJ:544:THR:HG21	18:CJ:552:ILE:N	1.36	1.34
18:CJ:484:HIS:HD2	18:CJ:495:ARG:NH1	1.17	1.33
18:CJ:544:THR:HG22	18:CJ:552:ILE:CG1	1.68	1.23

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DA	129/1788 (7%)	126 (98%)	3 (2%)	0	100	100
2	DL	139/307 (45%)	130 (94%)	9 (6%)	0	100	100
3	DB	1109/1181 (94%)	1078 (97%)	29 (3%)	2 (0%)	43	71
4	DC	1087/1165 (93%)	1052 (97%)	34 (3%)	1 (0%)	48	76
5	DE	576/747 (77%)	564 (98%)	11 (2%)	1 (0%)	43	71
6	DF	586/666 (88%)	569 (97%)	16 (3%)	1 (0%)	43	71
7	DG	558/631 (88%)	543 (97%)	14 (2%)	1 (0%)	43	71
8	DH	560/581 (96%)	540 (96%)	20 (4%)	0	100	100
9	DJ	313/396 (79%)	304 (97%)	8 (3%)	1 (0%)	36	64
10	DK	249/324 (77%)	240 (96%)	9 (4%)	0	100	100
11	DT	237/247 (96%)	233 (98%)	4 (2%)	0	100	100
12	DV	158/183 (86%)	151 (96%)	6 (4%)	1 (1%)	21	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	DW	159/179 (89%)	153 (96%)	6 (4%)	0	100	100
14	DX	139/169 (82%)	133 (96%)	6 (4%)	0	100	100
15	DY	152/163 (93%)	148 (97%)	4 (3%)	0	100	100
16	CC	72/74 (97%)	68 (94%)	3 (4%)	1 (1%)	9	31
17	CI	218/443 (49%)	210 (96%)	8 (4%)	0	100	100
18	CJ	796/817 (97%)	765 (96%)	30 (4%)	1 (0%)	48	76
19	CK	50/326 (15%)	47 (94%)	3 (6%)	0	100	100
20	CN	155/166 (93%)	150 (97%)	5 (3%)	0	100	100
21	CR	42/320 (13%)	40 (95%)	2 (5%)	0	100	100
22	CS	140/244 (57%)	135 (96%)	5 (4%)	0	100	100
23	Cg	480/498 (96%)	461 (96%)	19 (4%)	0	100	100
24	Ci	163/181 (90%)	155 (95%)	8 (5%)	0	100	100
25	Ck	699/874 (80%)	671 (96%)	26 (4%)	2 (0%)	36	64
All	All	8966/12670 (71%)	8666 (97%)	288 (3%)	12 (0%)	49	76

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	DJ	36	GLN
12	DV	57	THR
18	CJ	799	ASP
3	DB	1033	TYR
25	Ck	231	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DA	111/1514 (7%)	100 (90%)	11 (10%)	7	27
2	DL	123/263 (47%)	114 (93%)	9 (7%)	13	38
3	DB	976/1030 (95%)	855 (88%)	121 (12%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	DC	927/985 (94%)	803 (87%)	124 (13%)	4	15
5	DE	519/644 (81%)	454 (88%)	65 (12%)	4	17
6	DF	500/560 (89%)	433 (87%)	67 (13%)	4	15
7	DG	490/543 (90%)	427 (87%)	63 (13%)	4	16
8	DH	493/504 (98%)	427 (87%)	66 (13%)	4	15
9	DJ	275/347 (79%)	236 (86%)	39 (14%)	3	13
10	DK	209/261 (80%)	184 (88%)	25 (12%)	5	19
11	DT	220/228 (96%)	194 (88%)	26 (12%)	5	20
12	DV	145/165 (88%)	124 (86%)	21 (14%)	3	13
13	DW	148/163 (91%)	136 (92%)	12 (8%)	11	34
14	DX	124/149 (83%)	109 (88%)	15 (12%)	5	18
15	DY	137/146 (94%)	115 (84%)	22 (16%)	2	10
16	CC	73/73 (100%)	58 (80%)	15 (20%)	1	5
17	CI	186/370 (50%)	161 (87%)	25 (13%)	4	15
18	CJ	709/723 (98%)	616 (87%)	93 (13%)	4	16
19	CK	47/283 (17%)	39 (83%)	8 (17%)	2	9
20	CN	142/150 (95%)	122 (86%)	20 (14%)	3	13
21	CR	41/279 (15%)	32 (78%)	9 (22%)	1	4
22	CS	126/220 (57%)	108 (86%)	18 (14%)	3	13
23	Cg	424/437 (97%)	374 (88%)	50 (12%)	5	20
24	Ci	144/160 (90%)	124 (86%)	20 (14%)	3	14
25	Ck	608/747 (81%)	541 (89%)	67 (11%)	6	23
All	All	7897/10944 (72%)	6886 (87%)	1011 (13%)	6	16

5 of 1011 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	DH	9	THR
23	Cg	120	LEU
10	DK	116	ARG
23	Cg	57	THR
25	Ck	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 234 such sidechains are listed below:

Mol	Chain	Res	Type
8	DH	498	ASN
25	Ck	134	HIS
11	DT	219	GLN
25	Ck	113	ASN
23	Cg	296	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	CA	142/611 (23%)	85 (59%)	2 (1%)

5 of 85 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	CA	397	U
26	CA	398	U
26	CA	399	A
26	CA	400	U
26	CA	401	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	CA	512	G
26	CA	527	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GTP	Cg	501	32	33,34,34	0.94	1 (3%)	50,54,54	1.91	15 (30%)
29	SPD	DL	401	-	9,9,9	0.39	0	8,8,8	1.04	0
29	SPD	CA	703	-	9,9,9	0.39	0	8,8,8	0.58	0
30	UTP	DJ	401	-	29,30,30	1.74	8 (27%)	43,47,47	1.87	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GTP	Cg	501	32	-	5/22/38/38	0/3/3/3
29	SPD	DL	401	-	-	2/7/7/7	-
29	SPD	CA	703	-	-	5/7/7/7	-
30	UTP	DJ	401	-	-	13/22/38/38	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	DJ	401	UTP	PB-O3A	5.31	1.65	1.59
30	DJ	401	UTP	PA-O3A	2.44	1.62	1.59
30	DJ	401	UTP	PG-O3G	-2.28	1.46	1.54
30	DJ	401	UTP	PB-O3B	2.18	1.61	1.59
30	DJ	401	UTP	C6-C5	2.18	1.40	1.35

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Cg	501	GTP	C5-C4-N3	-5.01	120.42	128.39
31	Cg	501	GTP	O3G-PG-O3B	4.60	120.05	104.64
31	Cg	501	GTP	C2-N1-C6	-4.30	117.31	125.11
30	DJ	401	UTP	C4-N3-C2	-4.27	121.31	126.61
30	DJ	401	UTP	N3-C2-N1	4.16	120.31	114.89

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

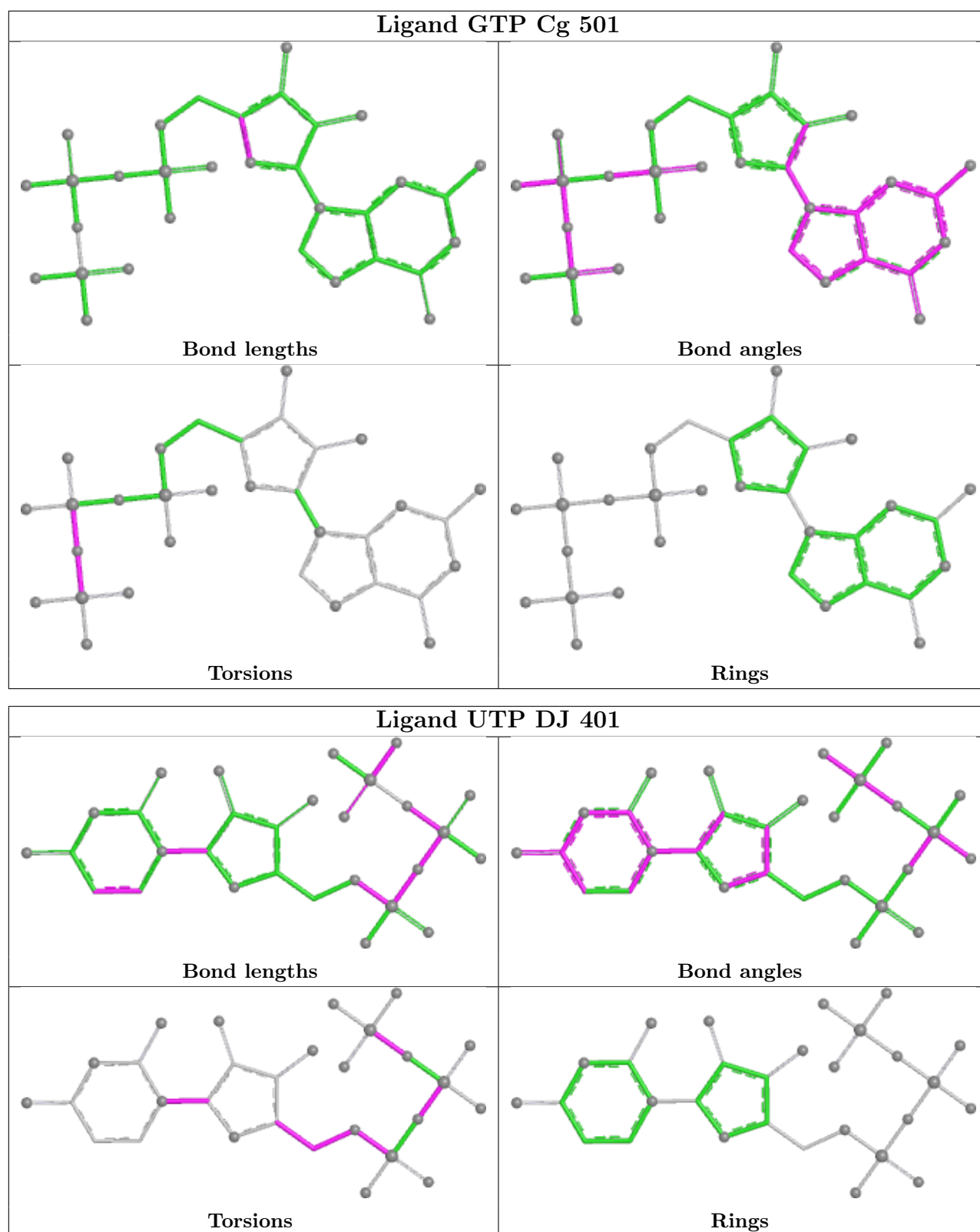
Mol	Chain	Res	Type	Atoms
30	DJ	401	UTP	C5'-O5'-PA-O1A
30	DJ	401	UTP	C5'-O5'-PA-O2A
30	DJ	401	UTP	O4'-C4'-C5'-O5'
31	Cg	501	GTP	PB-O3B-PG-O3G
29	CA	703	SPD	N6-C7-C8-C9

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	Cg	501	GTP	7	0
29	CA	703	SPD	2	0
30	DJ	401	UTP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

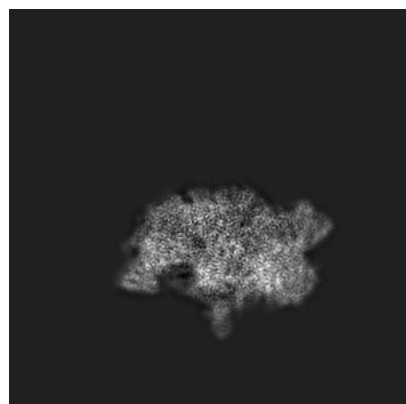
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0233. These allow visual inspection of the internal detail of the map and identification of artifacts.

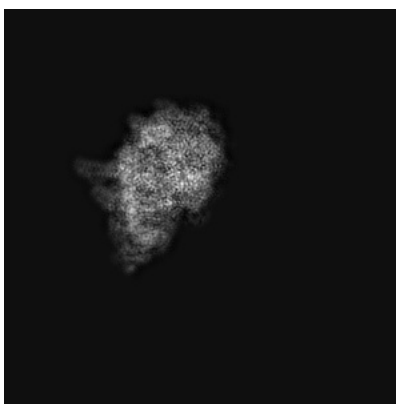
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

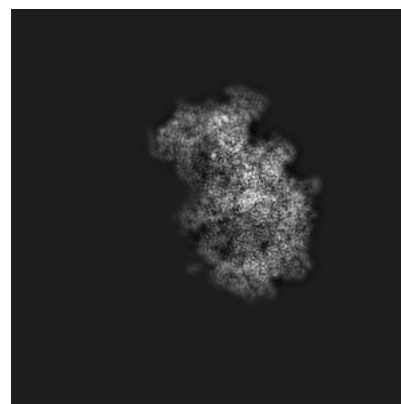
6.1.1 Primary map



X

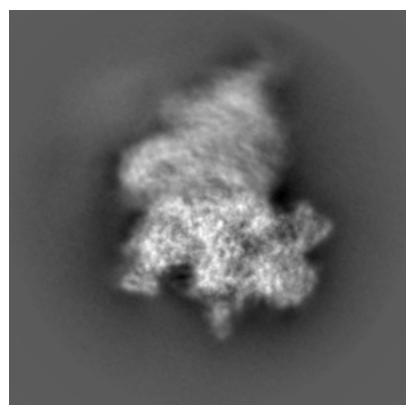


Y

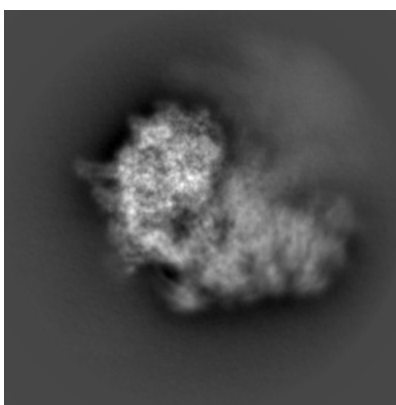


Z

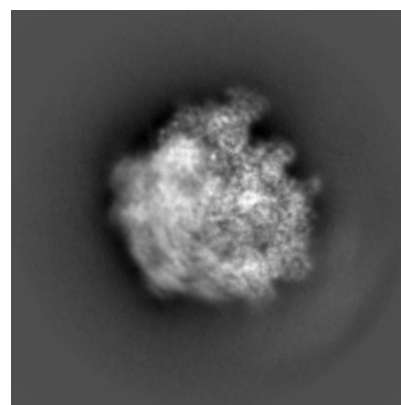
6.1.2 Raw map



X



Y

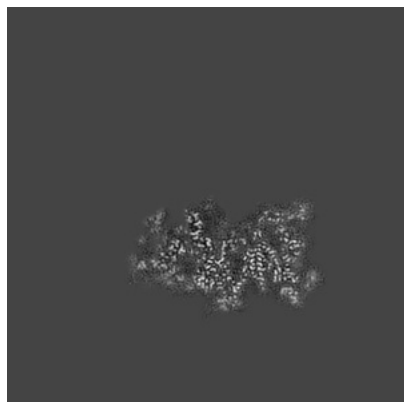


Z

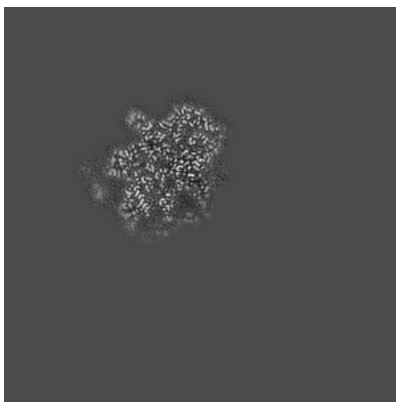
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

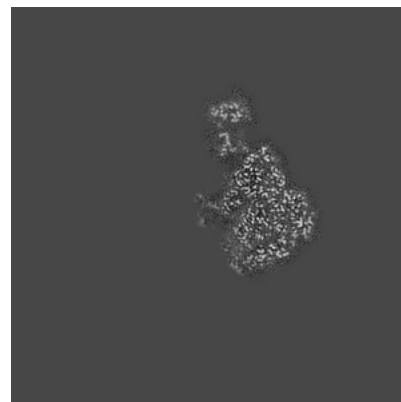
6.2.1 Primary map



X Index: 160

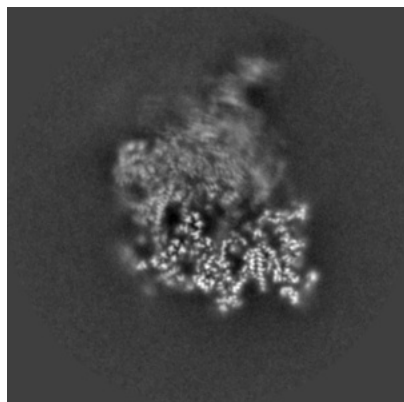


Y Index: 160

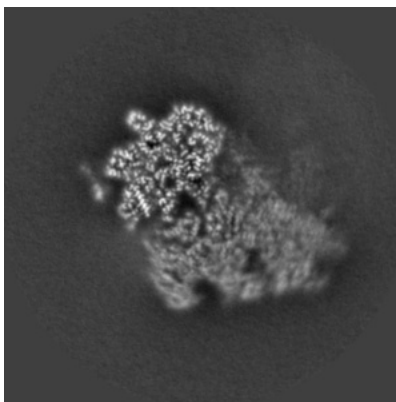


Z Index: 160

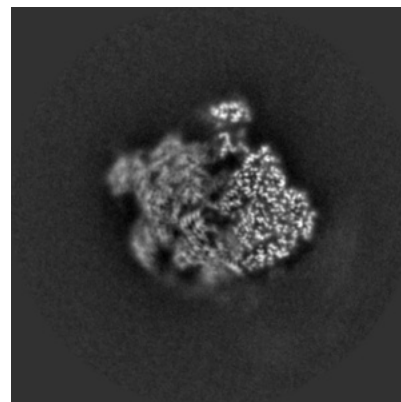
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

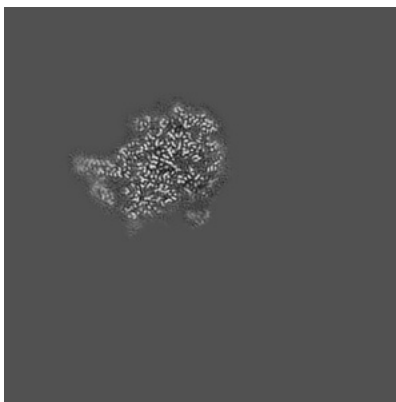
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

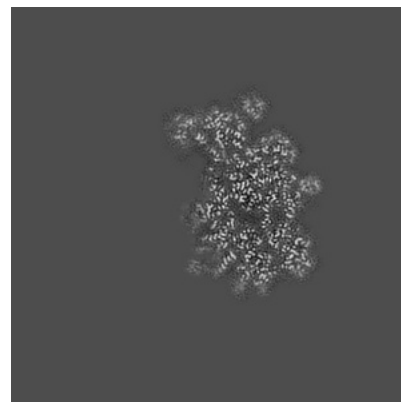
6.3.1 Primary map



X Index: 187

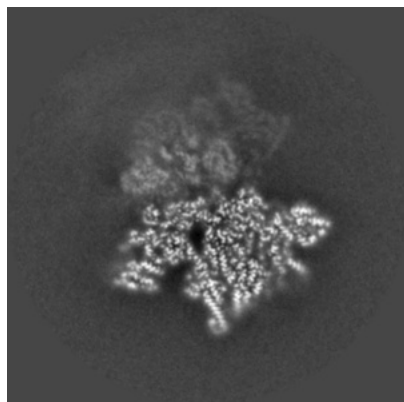


Y Index: 167

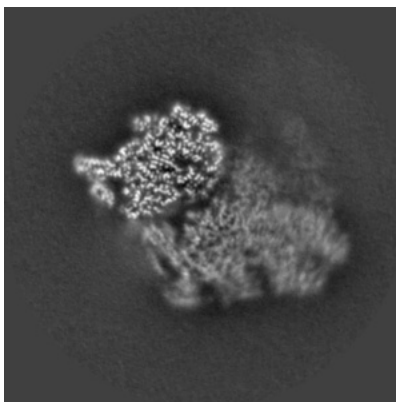


Z Index: 131

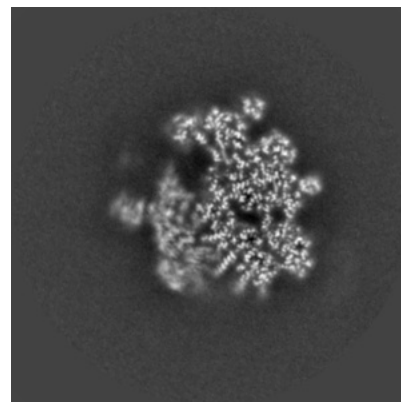
6.3.2 Raw map



X Index: 187



Y Index: 167

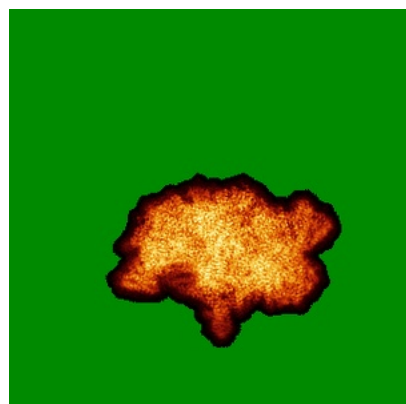


Z Index: 131

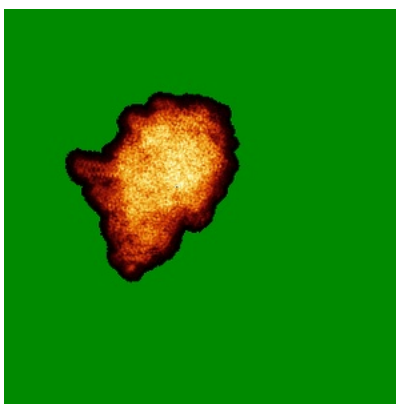
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

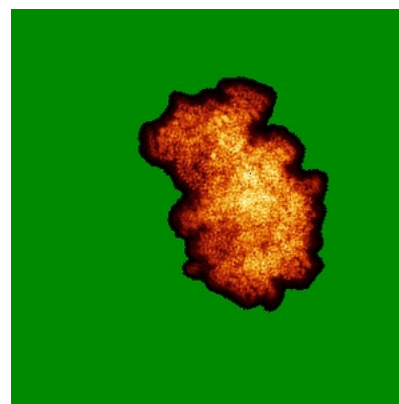
6.4.1 Primary map



X



Y

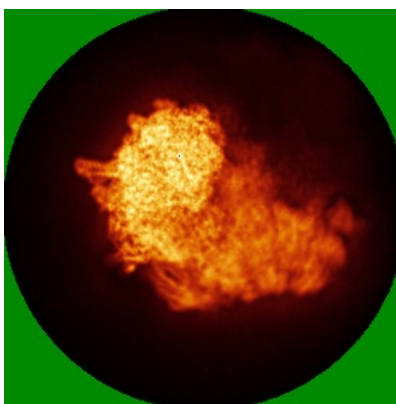


Z

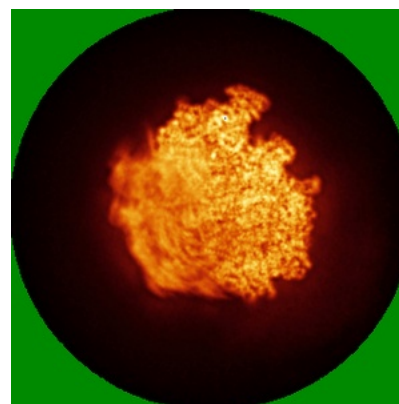
6.4.2 Raw map



X



Y

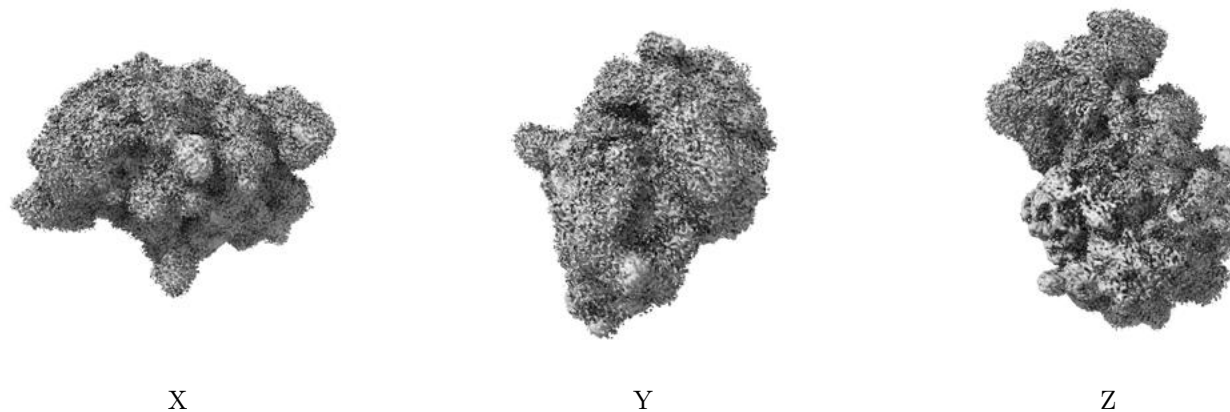


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

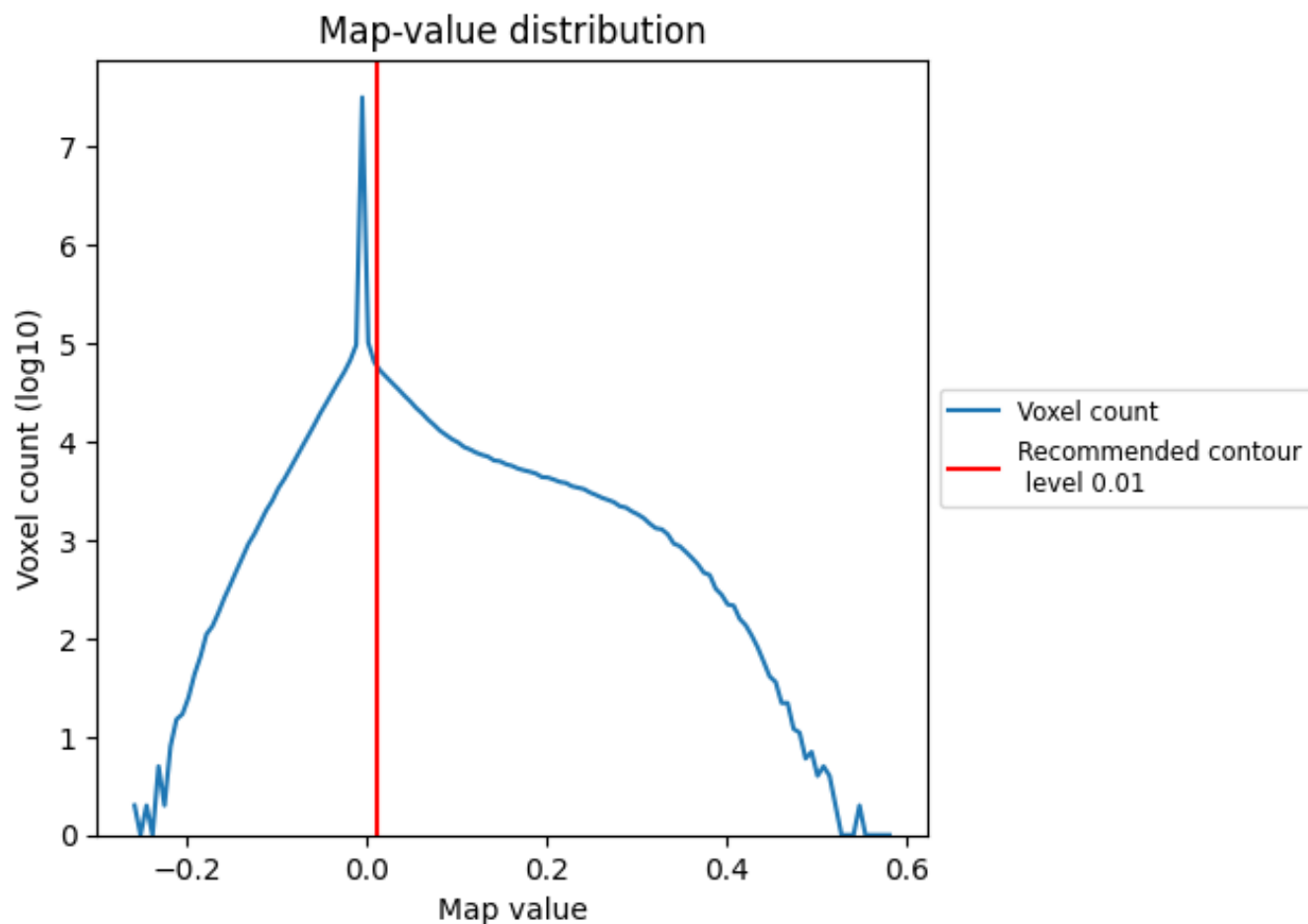
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

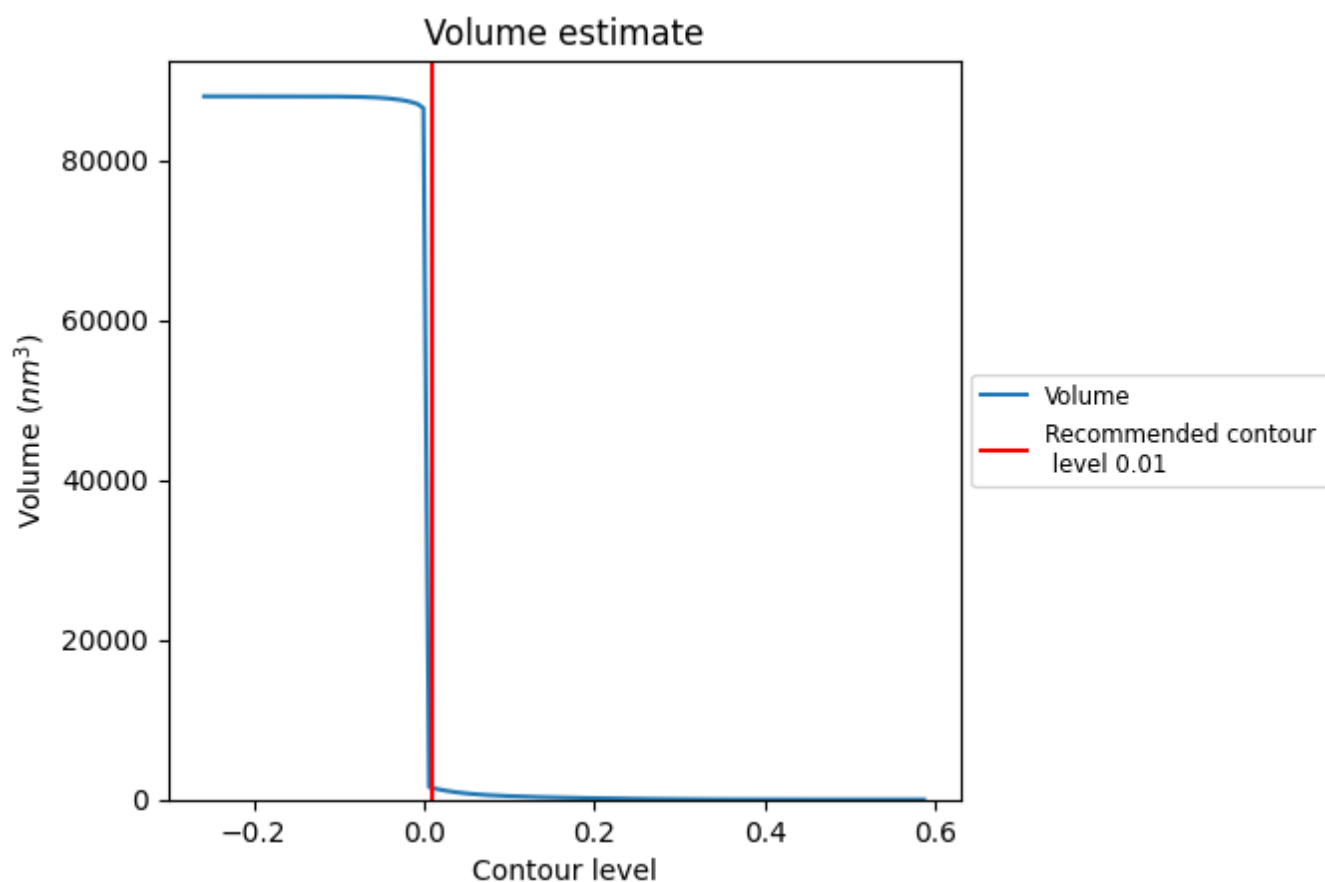
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

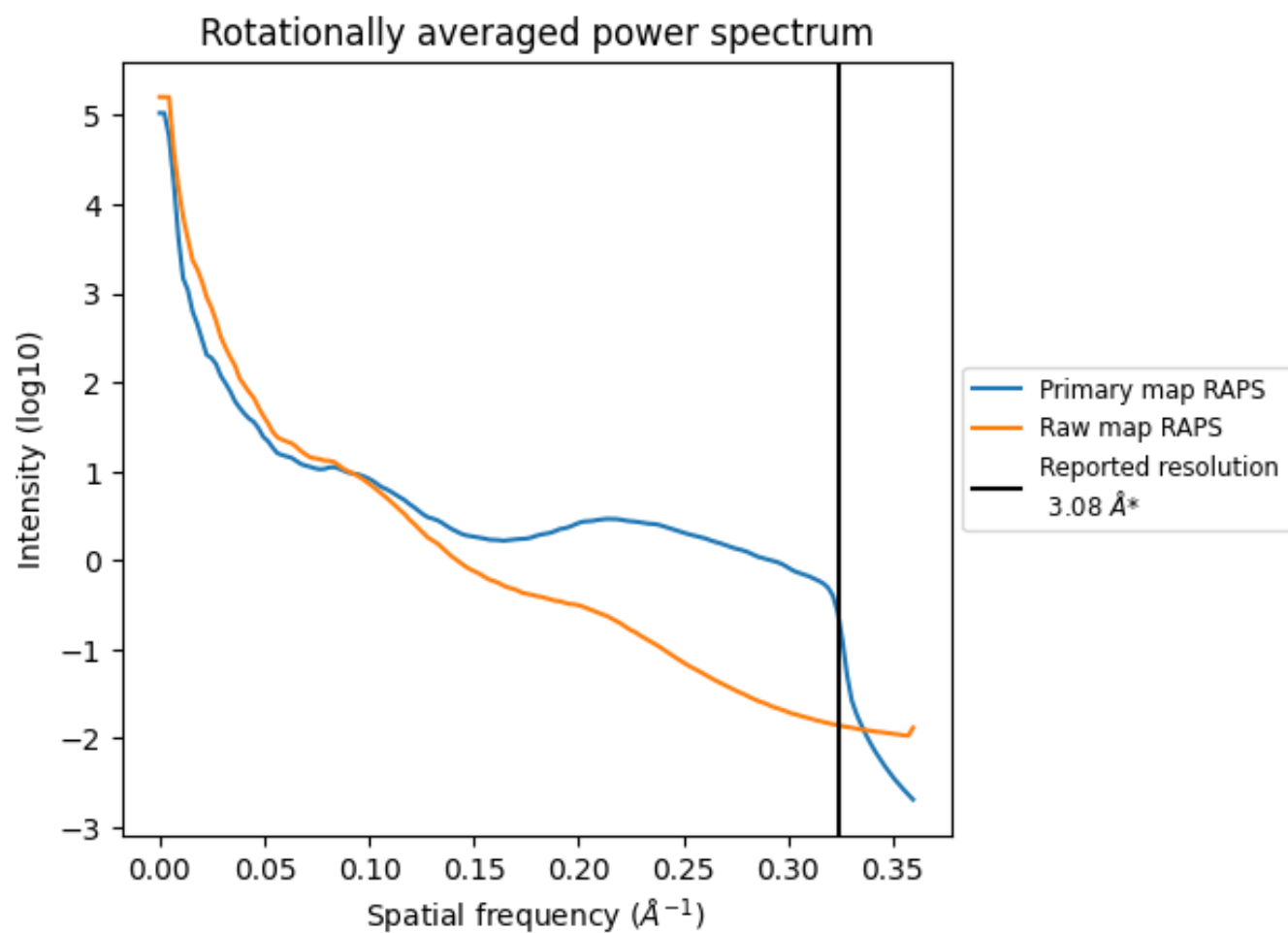
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1453 nm^3 ; this corresponds to an approximate mass of 1312 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

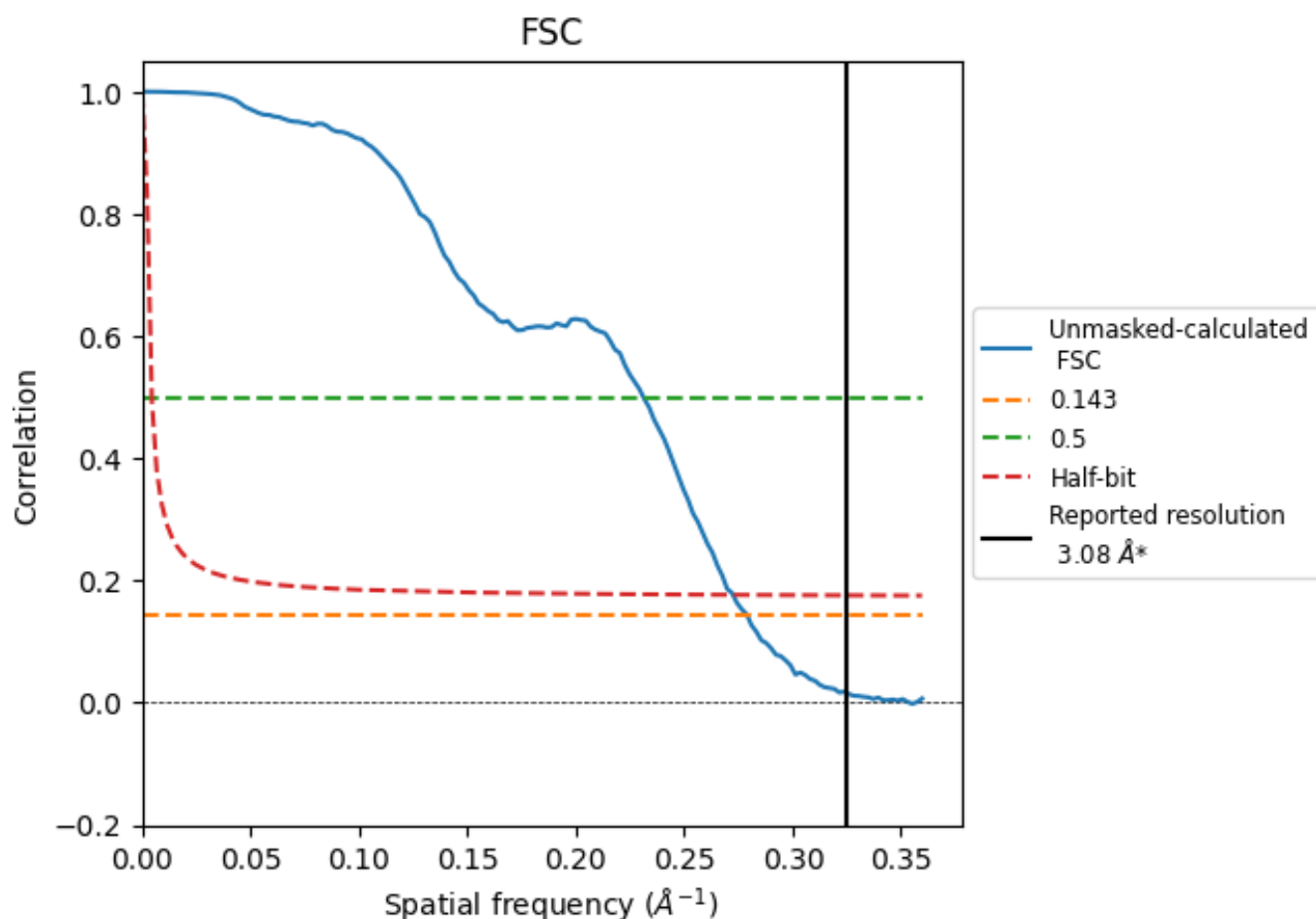


*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

8.2 Resolution estimates [i](#)

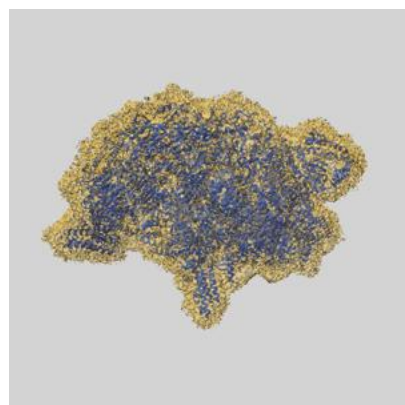
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	4.33	3.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.58 differs from the reported value 3.08 by more than 10 %

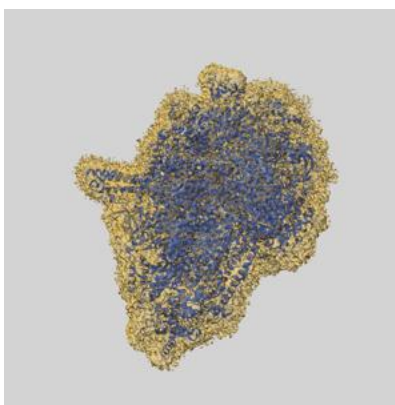
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0233 and PDB model 6HIZ. Per-residue inclusion information can be found in section [3](#) on page [15](#).

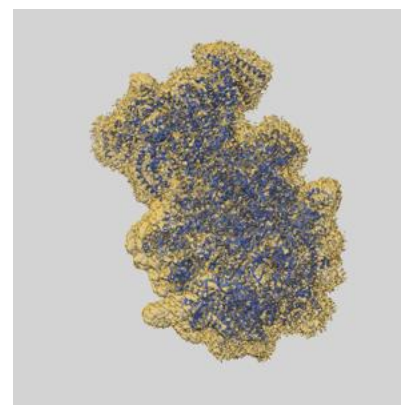
9.1 Map-model overlay [i](#)



X



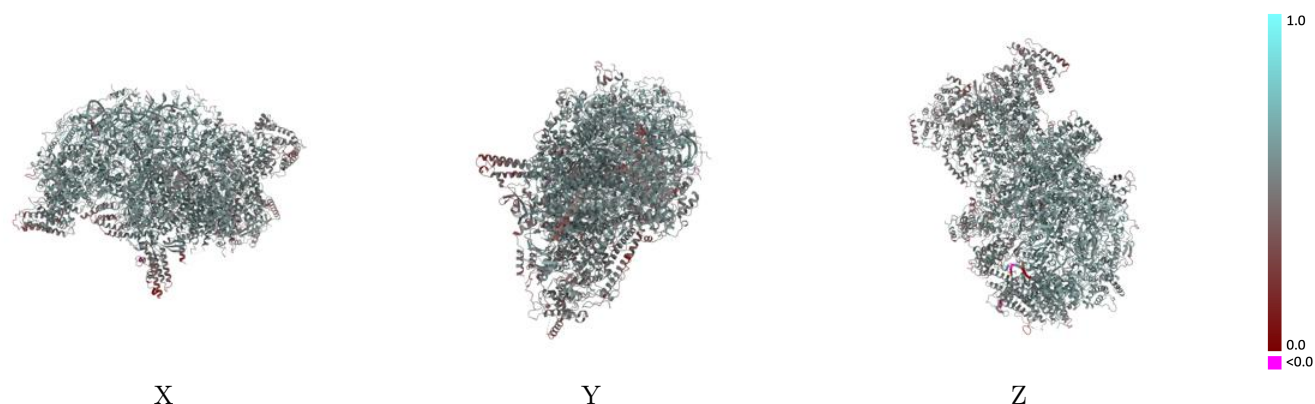
Y



Z

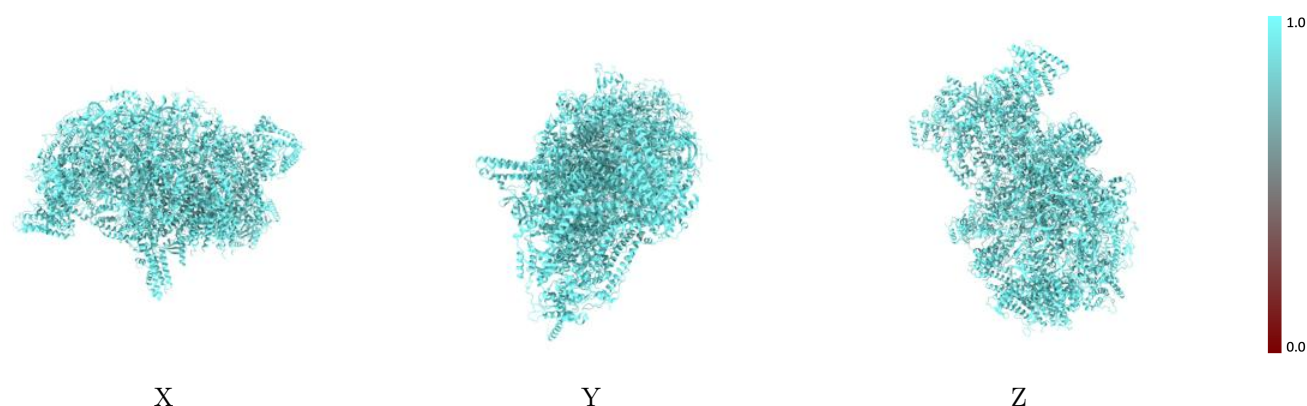
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



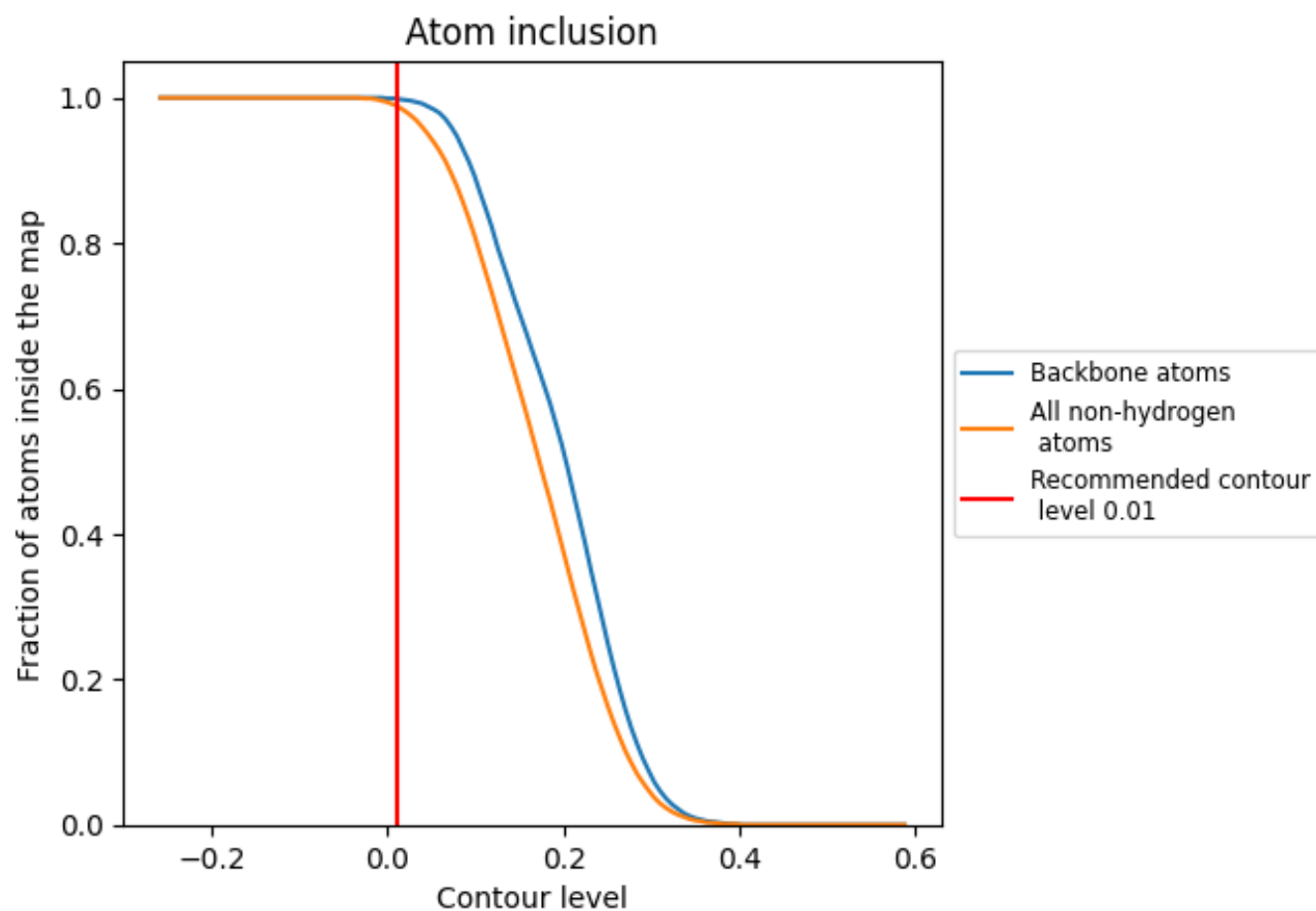
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9890	 0.5340
CA	 0.9940	 0.5550
CC	 0.9720	 0.5570
CI	 0.9860	 0.5660
CJ	 0.9880	 0.5560
CK	 0.9980	 0.5570
CN	 0.9940	 0.5830
CR	 0.9800	 0.5220
CS	 0.9940	 0.5730
Cg	 0.9940	 0.5550
Ci	 0.9890	 0.5670
Ck	 0.9860	 0.5040
DA	 0.9770	 0.4800
DB	 0.9830	 0.5310
DC	 0.9920	 0.4960
DE	 0.9930	 0.5000
DF	 0.9930	 0.5530
DG	 0.9910	 0.5060
DH	 0.9870	 0.5440
DJ	 0.9920	 0.5570
DK	 0.9890	 0.5270
DL	 0.9540	 0.5040
DT	 0.9930	 0.5690
DV	 0.9920	 0.5670
DW	 0.9900	 0.5550
DX	 0.9900	 0.5560
DY	 0.9950	 0.5700
UO	 1.0000	 0.5160
UP	 1.0000	 0.4590

